MODELING OF CHALCOGENIDE-BASED PHASE CHANGE MATERIALS

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We describe our effort to enable reliable atomistic simulations of the electro-thermally induced crystalline-amorphous, semiconducting-metallic phase transition in Te-based chalcogenide alloys. These alloys, of which GeTe is the basic archetype, can exhibit rapid switching and hold great potential for application as electronic devices, e.g., non-volatile memory elements. Reliable simulation of the phase transition requires quantum-like accuracy, but over a time scale only barely accessible to molecular dynamics (MD) with classical force fields (CFF). These CFF, in turn, must be capable of complex chemistry to model the rebonding that occurs in the phase transition, with Te being the critical substituent. We detail how to develop a viable CFF and inform semi-empirical quantum (tight-binding) MD based on first-principle quantum calculations. The detailed interplay of the different methods that operate with different length and time scales is critical to enabling meaningful simulations of GeTe, and the phase transition that makes this material interesting.